

Molière multiple scattering theory revisited

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Abstract

We have received rigorous relations between the exact and first-order parameters of the Molière multiple scattering theory, instead of the approximate one obtained in the original paper by Molière. We also estimated the corresponding Coulomb corrections to the Born approximation of the parameters and studied their Z dependence in the range of nuclear charge from $Z = 4$ to $Z = 82$. Additionally, we evaluated absolute and relative accuracies of the Molière theory in determining the screening angle and have concluded that for $Z \sim 80$ they are about 20 and 34 percents, respectively.

PACS: 11.80.La, 11.80.Fv, 32.80.Wr

Keywords: multiple scattering, approximations, Coulomb corrections

1 Introduction

The Molière multiple scattering theory of charged particles' [1, 2] is the most used tool for the multiple scattering effects accounting at experimental data processing. The experiment DIRAC [3] and many others [4-7] meets the problem of the excluding the multiple scattering effects in matter from obtained data. The standard theory of multiple scattering proposed by Molière and some its modifications [8-11] are used for this aim.

Estimation of the theory accuracy is of especial importance in the case of DIRAC experiment for it's high angular resolution. One of the significant

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sources of the inaccuracy of the Molière theory is the usage in [1, 2] an approximate relation for the exact and first-order values of the screening angle (χ_a) obtained in the original paper of Molière [1]:

$$\chi_a \approx \chi_a^B \sqrt{1 + 3.34 (Z\alpha/\beta)^2}, \quad (1)$$

since this parameter also determined other important quantities of the theory. In this connection, the problem of receiving the corresponding exact relation and estimating the Molière theory accuracy becomes important.

In the present work, we have obtained rigorous relations for a number of exact results of the theory and their Born approximations. We have also evaluated numerically the Coulomb corrections to the Born results and studied the Z -dependence of these corrections. In addition, we have estimated the absolute and relative accuracy of the Molière theory in determining the screening angle χ_a .

The outline of the paper is as follows. In Sec. 2-4 we review some basic results of [1, 2]. Namely, a solution of the transport equation (Sec. 2), the Molière expansion for this solution (Sec. 3), and determining the screening parameters by Molière (Sec. 4). The results of the present work are obtained in Sec. 5-6. In Sec. 5 we consider an another determination of the screening parameters allowing to receive rigorous relations between their exact and first-order values. In Sec. 6 we calculate the numerical values of the Coulomb corrections to the Born approximation in the range $Z = 4$ to $Z = 82$ and estimate the inaccuracy of the Molière theory. Finally, in Sec. 7 we summarize the main results of the paper. In Appendix we present an alternative way of obtaining the approximate solution of the transport equation for the thick targets. The some preliminary results of this work were announced in Refs. [12].

2 The transport equation and its solution

Let all scattering angles are small $\theta \ll 1$ so that $\sin \theta \sim \theta$, and the scattering problem is equivalent to diffusion in the plane of θ . Now let $\sigma(\chi)$ be the elastic differential cross section for the single scattering into the angular interval $\vec{\chi} = \vec{\theta} - \vec{\theta}'$, and $W_M(\theta, t)\theta d\theta$ is the number of scattered particles in the interval $d\theta$ after traversing a target thickness t . Then the transport equation is

$$\frac{\partial W_M(\theta, t)}{\partial t} = -n_0 W_M(\theta, t) \int \sigma(\chi) d^2\chi + n_0 \int W_M(\vec{\theta} - \vec{\chi}, t) \sigma(\chi) d^2\chi, \quad (2)$$

where $n_0 = eN_A/A$ is the number of the scattering atoms per cm^3 , N_A is the Avogadro number, and A is the atomic weight of the target atoms.

Moliere solved this equation for the determination of the spatial-angle distribution function $W_M(\theta, t)$ by the Fourier–Bessel method and gets to her a general expression

$$W_M(\theta, t) = \int_0^\infty J_0(\theta\eta) g(\eta, t) \eta d\eta, \quad (3)$$

in which

$$g(\eta, t) = \exp[N(\eta, t) - N_0(0, t)], \quad (4)$$

θ is the polar angle of the track of a scattering particle, measured with respect to the initial direction z ; η is the Fourier transform variable corresponding to θ ; and the Bessel function J_0 of order 0 is an approximate form for the Legendre polynomial appropriate to small scattering angles [2, 13].

In the notation of Molière

$$N(\eta, t) = 2\pi n_0 t \int_0^\infty \sigma(\chi) J_0(\chi\eta) \chi d\chi, \quad (5)$$

and N_0 is the value of (5) for $\eta = 0$, i.e. the total number of collisions

$$N_0(0, t) = 2\pi n_0 t \int_0^\infty \sigma(\chi) \chi d\chi. \quad (6)$$

The magnitude of $N_0 - N$ is much smaller than N_0 for values η , which are important, and may be called the ‘effective number of collisions’.

Inserting Eqs. (4)-(6) back into (3), we have

$$W_M(\theta, t) = \int_0^\infty \eta d\eta J_0(\theta\eta) \exp \left[-2\pi n_0 t \int_0^\infty \sigma(\chi) \chi d\chi [1 - J_0(\chi\eta)] \right]. \quad (7)$$

This equation is exact for any scattering law, provided only the angles are small compared with a radian.

At $g(\eta, 0) = 1$ for all η the expressions (3)-(6) can be rewritten as follows:

$$W_M(\theta, t) = \int_0^\infty J_0(\theta\eta) e^{-n_0 t Q(\eta)} \eta d\eta, \quad (8)$$

where

$$Q(\eta) = 2\pi \int_0^\infty \sigma(\chi)[1 - J_0(\chi\eta)]\chi d\chi. \quad (9)$$

This result is mathematically identical with result of Snyder and Scott for the distribution of projected angles [14].

3 The Molière expansion for the transport equations solution

One of the most important results of the Molière's theory is that the scattering is described by a single parameter, the so-called 'screening angle' (χ_a or χ'_a):

$$\chi'_a = \sqrt{1.167} \chi_a = [\exp(C_E - 0.5)] \chi_a \approx 1.080 \chi_a, \quad (10)$$

where $C_E = 0.57721$ is the Euler's constant.

More precisely, the angular distribution $W_M(\theta)\theta d\theta$ depends only on the ratio of the 'characteristic angle' χ_c , which describes the foil thickness, to the 'screening angle' which describes the scattering atom:

$$b = \ln \left(\frac{\chi_c}{\chi'_a} \right)^2 \equiv \ln \left(\frac{\chi_c}{\chi_a} \right)^2 + 1 - 2C_E \sim \ln N_0. \quad (11)$$

The screening angle χ_a can be determined approximately by the relation

$$\chi_a^2 \approx \chi_0^2 (1.13 + 3.76 a^2) = (\chi_a^B)^2 (1 + 3.34 a^2) \quad (12)$$

with the so-called 'Born parameter'

$$a = \frac{Ze^2}{\hbar v} = \frac{Z\alpha}{\beta}. \quad (13)$$

The second term in (12) represents the deviation from the Born approximation. If the value of this term is 0, the value of the screening angle is $\chi_a = \chi_a^B = \chi_0 \sqrt{1.13}$.

The angle χ_0 is defined by

$$\chi_0 = 1.13 \frac{Z^{1/3} m_e}{137 p} = \frac{Z^{1/3} m_e \alpha}{0.885 p}, \quad (14)$$

where $p = m_e v$ is momentum of incident particle and v is its velocity in the laboratory frame.

The characteristic angle is defined as

$$\chi_c^2 = 4\pi n_0 t \left(\frac{Z\alpha}{\beta p} \right)^2. \quad (15)$$

Its physical meaning is that the total probability of single scattering through an angle greater than χ_c is exactly one.

Putting $\chi_c \eta = y$ and setting $\theta/\chi_c = u$, for the most important values of η of order $1/\chi_c$, we get Molière's transformed equation

$$W_M(\theta)\theta d\theta = u du \int_0^\infty y dy J_0(uy) \exp \left\{ -\frac{y^2}{4} \left[b - \ln \left(\frac{y^2}{4} \right) \right] \right\}, \quad (16)$$

which is very much simpler in form than (7).

In order to obtain a result valid for large all angles, Molière defines the new parameter B by the transcendental equation

$$B - \ln B = b. \quad (17)$$

The angular distribution function can be written then as

$$W_M(\theta, B) = \frac{1}{\bar{\theta}^2} \int_0^\infty y dy J_0(\theta y) e^{-y^2/4} \exp \left[\frac{y^2}{4B} \ln \left(\frac{y^2}{4} \right) \right]. \quad (18)$$

The presented expansion method is to consider the term $[y^2 \ln(y^2/4)]/4B$ as a small parameter. Then the W_M is expanded in a power series in $1/B$:

$$W_M(\theta, t) = \sum_{n=0}^\infty \frac{1}{n!} \frac{1}{B^n} W_n(\theta, t) \quad (19)$$

with

$$W_n(\theta, t) = \frac{1}{\bar{\theta}^2} \int_0^\infty y dy J_0 \left(\frac{\theta}{\bar{\theta}} y \right) e^{-y^2/4} \left[\frac{y^2}{4} \ln \left(\frac{y^2}{4} \right) \right]^n, \quad (20)$$

$$\bar{\theta}^2 = \chi_c^2 B = 4\pi n_0 t \left(\frac{Z\alpha}{pv} \right)^2 B(t).$$

This method is valid for $B \geq 4.5$ and $\bar{\theta}^2 < 1$.

The first function $W_0(\theta, t)$ have simple analytical form:

$$W_0(\theta, t) = \frac{2}{\bar{\theta}^2} \exp\left(-\frac{\theta^2}{\bar{\theta}^2}\right), \quad (21)$$

$$\bar{\theta}^2 \underset{t \rightarrow \infty}{\sim} t \ln t. \quad (22)$$

For small angles, i.e. $\theta/\bar{\theta} = \theta/(\chi_c \sqrt{B}) = \Theta$ less than about 2, the Gaussian (21) is the dominant term. In this region, $W_1(\theta, t)$ is in general less than $W_0(\theta, t)$, so that the corrections to the Gaussian is of order of $1/B$, i.e. of order of 10%. An alternative way of obtaining the approximate solution (21) of (7) for the thick targets is given in Appendix.

A good approximate representation of the distribution at any angle is $W_0(\theta, t) + B^{-1}W_1(\theta, t)$, where

$$W_1(\theta, t) = \frac{2}{\bar{\theta}^2} \exp\left(-\frac{\theta^2}{\bar{\theta}^2}\right) \left\{ \left(\frac{\theta^2}{\bar{\theta}^2} - 1\right) \left[\overline{Ei}\left(\frac{\theta^2}{\bar{\theta}^2}\right) - \ln\left(\frac{\theta^2}{\bar{\theta}^2}\right) \right] + 1 \right\} - 2, \quad (23)$$

$\overline{Ei}(\Theta) = Ei(\Theta) + \pi i$, and $Ei(\Theta) = -\int_{-\Theta}^{\infty} e^{-t} \frac{dt}{t}$ is the exponential integral [15].

4 Molière's determination of the screening parameters

On the one hand, Molière writes the elastic Born cross section for the fast charged particle scattering in the atomic field as follows:

$$\sigma^B(\chi) = \sigma^R(\chi) \left(1 - \frac{F_A(p\chi)}{Z}\right)^2 = \sigma^R(\chi) q^B(\chi). \quad (24)$$

For angles χ small compared with a radian the exact Rutherford formula has a simple approximation:

$$\sigma^B(\chi) = \frac{\theta_c^2}{4\pi n_0 t (1 - \cos \chi)^2 \chi^4} q^B(\chi) \quad (25)$$

$$\approx \frac{\theta_c^2}{\pi n_0 t \chi^4} q^B(\chi). \quad (26)$$

Here, F_A is the atomic form factor and $q^B(\chi)$ is the ratio of actual to the Rutherford scattering cross sections in the Born approximation.

Then the screening angle χ_a^B in the Born approximation one can represent via F_A or $q^B(\chi)$ by the equations

$$-\ln(\chi_a^B) = \lim_{\varsigma \rightarrow \infty} \left[\int_0^{\varsigma} \left(1 - \frac{F_A(p\chi)}{Z} \right)^2 \frac{d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \quad (27)$$

$$= \lim_{\varsigma \rightarrow \infty} \left[\int_0^{\varsigma} \frac{q^B(\chi) d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \quad (28)$$

with an angle ς such as

$$\chi_0 \ll \varsigma \ll 1/\eta \sim \chi_c \quad (29)$$

and the angle $\chi_0 \sim m_e \alpha Z^{1/3}/p$.

Molière approximation for the Thomas—Fermi form factor $F_{T-F}(q)$ with momentum transfer q can be written as

$$F_{T-F}(q)^M = \sum_{i=1}^3 \frac{c_i \lambda_i^2}{q^2 + \lambda_i^2}, \quad (30)$$

in which

$$\begin{aligned} c_1 &= 0.35, & c_2 &= 0.55, & c_3 &= 0.10, \\ \lambda_1 &= 0.30\lambda, & \lambda_2 &= 4\lambda_1, & \lambda_3 &= 5\lambda_2. \end{aligned}$$

In the case where the Born parameter $a = 0$, the equation (27) for the screening angle can be evaluated directly, using the facts that $q(0) = 0$ and $\lim_{\varsigma \rightarrow \infty} q(\varsigma) = 1$. Then with use of (24) and (30) can also be obtained the following approximation for $(\chi_a')^B$ [1, 14]:

$$(\chi_a')^B = [\exp(C_E - 0.5)] \frac{\lambda}{p} A = \sqrt{1.174} \chi_0 A, \quad (31)$$

where $\lambda = m_e \alpha Z^{1/3}/0.885$. We should note that in Refs. [1, 14] admitted a misprint, namely, the factor $A = 1.0825$ in Eq. (31) should be replaced by $A = 1.065 = \sqrt{1.13}$.

On the other hand, Molière writes the nonrelativistic Born cross section in the form

$$\sigma^B(\chi) = k^2 \left| \int_0^\infty \rho d\rho J_0 \left(2k\rho \sin \frac{\chi}{2} \right) \Phi_M^B(\vec{\rho}) \right|^2 \quad (32)$$

where the Born phase shift is given in units of $\hbar = c = 1$ by

$$\Phi_M^B(\vec{\rho}) = -\frac{2}{v} \int_{\rho}^{\infty} \frac{U_{\lambda}(r) dr}{\sqrt{r^2 - \rho^2}} = -\frac{1}{v} \int_{-\infty}^{\infty} U_{\lambda} \left(r = \sqrt{\rho^2 + z^2} \right) dz. \quad (33)$$

Here, k is the wave number of the incident particle, the variable ρ corresponds to the impact parameter of the collision, and $U_{\lambda}(r)$ is the screened Coulomb potential of the target atom

$$U_{\lambda}(r) = \pm Z \frac{\alpha}{r} \Lambda(\lambda r) \quad (34)$$

with Molière's fit to the Thomas—Fermi screening function $\Lambda(\lambda r)$

$$\Lambda(\lambda r) \simeq 0.1e^{-6\lambda r} + 0.55e^{-1.2\lambda r} + 0.35e^{-0.3\lambda r}. \quad (35)$$

In order to obtain a result valid for large a (i.e. not restricted to the Born approximation) and also for large angles χ (up to 90° and beyond), Molière uses in his calculations of the screening angle a WKB technique.

We point out that the value of χ_a will depend both on screening properties of atom, and on $\sigma(\chi)$ -approximation used for its calculation.

The exact formulas for the WKB differential cross section $\sigma(\chi)$ and corresponding $q(\chi)$ in terms of an integral are given in Molière's paper [1] as follows:

$$\sigma(\chi) = k^2 \left| \int_0^{\infty} \rho d\rho J_0(k\chi\rho) \left\{ 1 - \exp [i\Phi_M(\vec{\rho})] \right\} \right|^2, \quad (36)$$

$$q(\chi) = \frac{(k\chi)^4}{4a^2} \left| \int_0^{\infty} \rho d\rho J_0(k\chi\rho) \left\{ 1 - \exp [i\Phi_M(\vec{\rho})] \right\} \right|^2 \quad (37)$$

with the phase shift given by

$$\Phi_M(\vec{\rho}) = \int_{-\infty}^{\infty} [k_r(r) - k] dz, \quad (38)$$

where $k_r(r)$ is the relativistic wavenumber for the particle at a distance r from the nucleus, and the quantity ρ is seen to be impact parameter of the trajectory or 'ray'. As before, k is the initial or asymptotic value of the wavenumber.

When $k_r(r)$ is expanded as a series of powers of $U_\lambda(r)/k$, then the first-degree term yields the same expression for $\Phi_M(\vec{\rho})$ as Eq. (33). The Born approximation for (36) is obtained by expanding the exponential in (36) to first order in parameter a (13).

Relations (26) and (28) between the quantities $\sigma^B(\chi)$, $q^B(\chi)$, and χ_a^B remain valid also for $\sigma(\chi)$, $q(\chi)$, and χ_a .

Despite the fact that the formulas (36), (37) are exact, evaluation of these quantities was carried out by Moliere only approximately.

To estimate (37), Molière used the first-order Born shift (33) with (34) and (35), what is good only to terms of first order in a , and found

$$q(\chi) \approx \left| 1 - \frac{4ia(1-ia)^2}{(\chi/\chi_0)^2} \left\{ -0.81 + 2.21 \left[-\Re[\psi(ia)] - \frac{1}{1-ia} + \frac{1}{2ia} + \lg \frac{\chi}{2\chi_0} \right] \right\} \right|^2. \quad (39)$$

Here, ψ is the so-called ‘digamma function’, i.e. the logarithmic derivative of the Γ -function $\psi(x) = d \ln \Gamma(x)/dx$.

He has fitted a simple formula to the function $\Re[\psi(ia)]$ in Eq. (39)

$$\Re[\psi(ia)] \approx \frac{1}{4} \lg \left(a^4 + \frac{a^2}{3} + 0.13 \right). \quad (40)$$

Using (40) in Eq. (39) and expanding with neglect of higher orders in a^2 and $(\chi/\chi_0)^{-2}$, he got

$$q(\chi) \approx 1 - \frac{8.85}{(\chi/\chi_0)^2} \left[1 + 2.303 a^2 \lg \frac{7.2 \cdot 10^{-4} (\chi/\chi_0)^4}{(a^4 + a^2/3 + 0.13)} \right]. \quad (41)$$

Molière has calculated $q(\chi)$ for different values of a and as a result has devised an interpolation scheme, based on a linear relation between $(\chi/\chi_0)^2$ and a^2 for fixed q :

$$(\chi/\chi_0)^2 \approx A_q + a^2 B_q. \quad (42)$$

Calculating the screening angle defined by

$$-\ln(\chi_a) = \frac{1}{2} + \lim_{\varsigma \rightarrow \infty} \left[\int_0^\varsigma \frac{q(\chi) d\chi}{\chi} - \ln \varsigma \right] = \frac{1}{2} - \ln \chi_0 - \int_0^1 dq \ln \left(\frac{\chi}{\chi_0} \right) \quad (43)$$

and assuming a linear relation between χ_a^2 and a^2 , Molière writes finally the following interpolating formula:

$$\chi_a \approx \chi_0 \sqrt{1.13 + 3.76 a^2}. \quad (44)$$

Critical remarks to his conclusion see in the review of V.T. Scott [14].

5 An alternative determining the screening parameters

To obtain an exact correction to the first-order Born screening angle $(\chi'_a)^B$, we will carry out our analytical calculation in terms of the function $Q_{el}(\eta)$ (9):

$$Q(\eta) = 2\pi \int_0^\infty \sigma(\chi)[1 - J_0(\chi\eta)]\chi d\chi \equiv \int d^2\rho \left[1 - \cos[\Delta\Phi(\vec{\rho}, \vec{\eta})], \right] \quad (45)$$

where the phase shift is determined by the equation

$$\Delta\Phi(\vec{\rho}, \vec{\eta}) = \Phi(\rho_+) - \Phi(\rho_-), \quad \vec{\rho}_\pm = \vec{\rho} \pm \vec{\eta}/2p. \quad (46)$$

Substituting the expression for the cross section

$$\sigma(\chi) = \frac{\chi_c^2}{\pi n_0 t \chi^4} q(\chi) \quad (47)$$

into (45), we rewrite it in the form:

$$n_0 t Q(\eta) = 2\chi_c^2 \int_0^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi. \quad (48)$$

For the important values of η of order $1/\chi_c$ or less, it is possible to split the last integral at the angle ς (29) into two integrals:

$$\begin{aligned} I(\eta) &= \int_0^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi \\ &= \int_0^\varsigma [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi + \int_\varsigma^\infty [1 - J_0(\chi\eta)] q(\chi) \chi^{-3} d\chi \\ &= I_1(\varsigma\eta) + I_2(\varsigma\eta). \end{aligned} \quad (49)$$

For the part from 0 to ς , we may write $1 - J_0(\chi\eta) = \chi^2\eta^2/4$, and the integral I_1 reduces to a universal one, independently of η :

$$I_1(\varsigma\eta) = \frac{\eta^2}{4} \int_0^\varsigma q(\chi) d\chi/\chi. \quad (50)$$

For the part from ς to infinity, the quantity $q(\chi)$ can be replaced by unity and the integral I_2 can be integrated by parts. This leads to the following result for I_2 :

$$I_2(\varsigma\eta) = \frac{\eta^2}{4} \left[1 - \ln(\varsigma\eta) + \ln 2 - C_E + O(\varsigma\eta) \right]. \quad (51)$$

Integrating (50) with the account (43), substituting obtained solutions back into (48), and also using definition

$$\ln(\chi_c/\chi_a)^2 + 1 - 2C_E = \ln(\chi_c/\chi'_a)^2,$$

as a result for $Q(\eta)$ we obtain:

$$\begin{aligned} Q(\eta) &= -\frac{(\chi_c\eta)^2}{2n_0t} \left[\ln\left(\frac{\chi_c^2\eta^2}{4}\right) - \ln\left(\frac{\chi_c}{\chi'_a}\right)^2 \right] \\ &= -\frac{(\chi_c\eta)^2}{2n_0t} \ln\left(\frac{\eta^2(\chi'_a)^2}{4}\right). \end{aligned} \quad (52)$$

Finally, considering definition of θ_c (15), we can represent $Q(\eta)$ by the following expression:

$$Q(\eta) = -2\pi \left(\frac{Z\alpha}{\beta p}\right)^2 \eta^2 \ln\left(\frac{\eta^2(\chi'_a)^2}{4}\right). \quad (53)$$

Then, the screening angle χ'_a can be determined via $Q(\eta)$ by a linear equation:

$$-\ln(\chi'_a)^2 = \ln\left(\frac{\eta^2}{4}\right) + \left[2\pi\eta^2 \left(\frac{Z\alpha}{\beta p}\right)^2 \right]^{-1} Q(\eta). \quad (54)$$

Let us present the quantity $Q_{el}(\eta)$ in the form:

$$Q(\eta) = Q^B(\eta) - \Delta_{CC}[Q(\eta)]. \quad (55)$$

Then, on the one hand, using (53), the difference $\Delta_{CC}[Q(\eta)]$ between the Born approximate $Q^B(\eta)$ and exact in the Born parameter values of the quantity $Q(\eta)$ can be reduced to a difference in the quantities $\ln(\chi'_a)$ and $\ln(\chi'_a)^B$:

$$\begin{aligned} \Delta_{CC}[Q(\eta)] &\equiv Q^B(\eta) - Q(\eta) \\ &= 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p}\right)^2 \left[\ln(\chi'_a) - \ln(\chi'_a)^B \right] \equiv 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p}\right)^2 \Delta_{CC}[\ln(\chi'_a)]. \end{aligned}$$

On the other hand, this difference can be reduced to a difference $\Delta q(\chi) = q^B(\chi) - q(\chi)$:

$$\Delta_{CC}[Q(\eta)] = 2\pi \int_0^\infty \chi d\chi \Delta\sigma(\chi) [1 - J_0(\chi\eta)] = \frac{2\chi_c^2}{n_0 t} \int_0^\infty \frac{d\chi}{\chi^3} \Delta q(\chi) [1 - J_0(\chi\eta)], \quad (56)$$

and for (37) with (46), as a result of integration, (56) becomes

$$\Delta_{CC}[Q(\eta)]_{\eta \rightarrow 0} = 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p} \right)^2 \left[\frac{1}{2} \psi \left(i \frac{Z\alpha}{\beta} \right) + \frac{1}{2} \psi \left(-i \frac{Z\alpha}{\beta} \right) - \psi(1) \right] \quad (57)$$

$$= 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p} \right)^2 \left\{ \Re \left[\psi \left(1 + i \frac{Z\alpha}{\beta} \right) \right] + C_E \right\}, \quad (58)$$

where

$$\begin{aligned} \Re[\psi(1 + ia)] &= \Re[\psi(1 - ia)] = \Re[\psi(ia)] = \Re[\psi(-ia)] \\ &= -C_E + a^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + a^2)} = -C_E + f(a), \end{aligned} \quad (59)$$

$$-\infty < a < \infty,$$

$\psi(1) = -C_E$, and $f(a) = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}$ is an ‘universal function of $a = Z\alpha/\beta$ ’.

As consequence, we can get the following rigorous relations between the quantities $\ln(\chi'_a)$ and $\ln(\chi'_a)^B$:

$$\ln(\chi'_a) - \ln(\chi'_a)^B = \Re[\psi(1 + ia) - \psi(1)], \quad (60)$$

$$\Delta_{CC}[\ln(\chi'_a)] = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}. \quad (61)$$

We point out that the relations (58), (60), and (61) are independent on the form of electron distribution in atom and are valid for any atomic model.

From (58) also follows an expression for the correction to the exponent of (7). Since $\ln[g(\eta)] = -n_0 t Q$, we get:

$$\Delta_{CC}[\ln g(\eta)] \equiv \ln[g(\eta)] - \ln[g^B(\eta)] \quad (62)$$

$$= 4\pi\eta^2 n_0 t \left(\frac{Z\alpha}{\beta p} \right)^2 f(a).$$

For the specified value of $\eta^2 = 1/\chi_c^2$, using the definition of χ_c (15), we can evaluate this correction:

$$\Delta_{CC}[\ln g(\chi_c)] = \frac{4\pi n_0 t}{\chi_c^2} \left(\frac{\chi_c^2}{4\pi n_0 t} \right)^2 f(a) = f(a). \quad (63)$$

The formulas for the so-called ‘Coulomb correction’ (CC), defined as a difference between the exact and the Born approximate results, are known as the Bethe—Bloch formulas for the ionization losses [16] and the formulas for the Bethe—Heitler cross section of bremsstrahlung [17]¹. The similar expression was found for the total cross section of the Coulomb interaction of compact hadronic atoms with ordinary target atoms [19]. Were also obtained CC to the cross sections of the pair production in nuclear collisions [20, 21] as well as to the solutions of the Dirac and Klein-Gordon equations [22]. Specificity of the expressions received in the present work is that they define CC not to the cross sections of the processes, but to screening angle and an exponential part of the distribution function.

6 Relative Coulomb corrections to the Born approximation

Let us write (61) in the following way

$$(\chi'_a) = (\chi'_a)^B \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right]. \quad (64)$$

The exact (Coulomb) relative corrections to the Born screening angle $(\chi'_a)^B$ can be then represented as

$$\delta_{CC}(\chi'_a) = \frac{\chi'_a - (\chi'_a)^B}{(\chi'_a)^B} = \frac{\Delta(\chi'_a)}{(\chi'_a)^B} = \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right] - 1. \quad (65)$$

The relative CC to the exponent $g^B(\eta)$ at $\eta^2 = 1/\chi_c^2$, as follows from (63), is also determined by this quantity, $\delta_{CC}(\chi'_a) = \delta_{CC}[g(\chi_c)]$. Moreover, because

$$\Delta W(\chi_c, t) \equiv W_M - W_M^B = \int_0^\infty J_0(\theta\eta) \Delta g(\chi_c) \eta d\eta, \quad (66)$$

accounting $\int_0^\infty d\eta \eta J_0(\theta\eta) = 0$, we get

¹ The more complicate formal expression for CC was derived by I. Øverbø in [18].

$$\delta_{CC} [W_M(\chi_c, t)] = \frac{\Delta W(\chi_c, t)}{W^B(\chi_c, t)_M} = \frac{\Delta g(\chi_c)}{g^B(\chi_c)} = \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right] - 1. \quad (67)$$

Thus,

$$\delta_{CC} \equiv \delta_{CC}(\chi'_a) = \delta_{CC} [g(\chi_c)] = \delta_{CC} [W_M(\chi_c, t)].$$

Note also that from the Molière equation (39) and to it equivalent

$$q(\chi) \approx 1 - \frac{8.85}{(\chi/\chi_0)^2} \left\{ 1 + 4a^2 \left[\lg \left(\frac{\chi}{2\chi_0} \right) - f \left(\frac{Z\alpha}{\beta} \right) - 0.543 \right] \right\} \quad (68)$$

ensues an approximate expression for the relative correction of exact to the Rutherford cross section $\delta(\sigma) = (\sigma - \sigma^R)/\sigma^R$:

$$\delta(\sigma) \approx \frac{8.85}{(\chi/\chi_0)^2} \left\{ 1 + 4a^2 \left[\lg \left(\frac{\chi}{2\chi_0} \right) - f \left(\frac{Z\alpha}{\beta} \right) - 0.543 \right] \right\}. \quad (69)$$

The expression in the inner brackets is close in its form to the inner parts of the Bethe—Bloch [16], Bethe-Maximon [17] formulas, and also formula for the total cross section from [19].

To compare the second-order relative corrections to the first-order results ($\delta_{CC}^{(2)}$ and $\delta_M^{(2)}$), which correspond to Eqs. (64) and (12), respectively, and to investigate their Z -dependence, we first present these equations in the following approximate form:

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right], \quad (70)$$

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right]. \quad (71)$$

The last expression follows from

$$\chi_a \approx \chi_a^B \sqrt{1 + 3.34 \left(\frac{Z\alpha}{\beta} \right)^2} \approx \chi_a^B \left[1 + 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right], \quad (72)$$

where $\chi_a = (\chi'_a)/1.080$ and $\chi_a^B = (\chi'_a)^B/1.080$. Then, (70) and (71) becomes

$$\delta_{CC}^{(2)}(\chi'_a) \approx \frac{\Delta(\chi'_a)}{(\chi'_a)^B} \approx 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right), \quad (73)$$

$$\delta_M^{(2)}(\chi'_a) \approx \frac{\Delta(\chi'_a)}{(\chi'_a)^B} \approx 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right). \quad (74)$$

Additionally, in order to assess the accuracy of the Molière theory in determining the screening angle χ'_a , we also define the absolute and relative differences between the values of $\delta_M^{(2)}(\chi'_a)$ and $\delta_{CC}^{(2)}(\chi'_a)$ as well as between the $\delta_M^{(2)}(\chi'_a)$ and $\delta_{CC}(\chi'_a)$ by the relations

$$\delta_{CCM}^{(2)}(\chi'_a) = \frac{\Delta_{CCM}^{(2)}(\chi'_a)}{\delta_M^{(2)}} = \frac{\delta_M^{(2)} - \delta_{CC}^{(2)}}{\delta_M^{(2)}} = 1 - \frac{\delta_{CC}^{(2)}}{\delta_M^{(2)}}, \quad (75)$$

$$\delta_{CCM}(\chi'_a) = \frac{\Delta_{CCM}(\chi'_a)}{\delta_M^{(2)}} = \frac{\delta_M^{(2)} - \delta_{CC}}{\delta_M^{(2)}} = 1 - \frac{\delta_{CC}}{\delta_M^{(2)}}. \quad (76)$$

Table 1 presents the Z dependence of the second-order corrections to the first-order results. It shows that the values of the relative corrections $\delta_{CC}^{(2)}$ for heavy target atoms with $Z \sim 80$ does reach 40%. From it is also obvious that with the rise in the nuclear charge the absolute inaccuracy $\Delta_{CCM}^{(2)}(\chi'_a)$ of the Molière's theory in determining the screening angle χ'_a increases to approximately 16%, and the corresponding relative error $\delta_{CCM}^{(2)}(\chi'_a)$ does not depend on Z and is about 28%.

Table 1. The Z dependence of the second-order corrections defined by Eqs. (73)–(75)

M	Z	$Z\alpha$	$\delta_{CC}^{(2)}$	$\delta_M^{(2)}$	$\Delta_{CCM}^{(2)}$	$\delta_{CCM}^{(2)}$
Be	4	0.029	0.001	0.001	0.000	0.286
Al	13	0.094	0.011	0.015	0.004	0.280
Ti	22	0.160	0.031	0.043	0.012	0.280
Ni	28	0.204	0.050	0.070	0.020	0.286
Mo	42	0.307	0.113	0.157	0.044	0.280
Sn	50	0.365	0.160	0.222	0.062	0.279
Ta	73	0.533	0.342	0.474	0.132	0.278
Pt	78	0.569	0.390	0.541	0.150	0.279
Au	79	0.577	0.400	0.554	0.154	0.278
Pb	82	0.598	0.431	0.598	0.166	0.279

We can also calculate the exact ('Coulomb') corrections according to the formulas (61), (65) and compare them with the results of the calculation of Molière, using (76) (Table 2). For this purpose, we must first calculate the values of the function $f(a) = \Re[\psi(1 + ia)] + C_E$.

Table 2. The Z dependence of the exact corrections, defined by Eqs. (61), (65), and (76)

M	Z	$Z\alpha$	Σ	$f(Z\alpha)$	δ_{CC}	Δ_{CCM}	δ_{CCM}
Be	4	0.029	1.2012	0.0010	0.001	0.000	0.286
Al	13	0.094	1.1928	0.0107	0.011	0.004	0.280
Ti	22	0.160	1.1758	0.0306	0.031	0.012	0.280
Ni	28	0.204	1.1602	0.0487	0.050	0.020	0.287
Mo	42	0.307	1.1127	0.1046	0.110	0.047	0.297
Sn	50	0.365	1.0799	0.1436	0.154	0.068	0.306
Ta	73	0.533	0.9710	0.2758	0.318	0.157	0.330
Pt	78	0.569	0.9467	0.3067	0.359	0.182	0.336
Au	79	0.577	0.9414	0.3125	0.367	0.187	0.337
Pb	82	0.598	0.9263	0.3316	0.393	0.205	0.342

From the digamma series

$$\psi(1+a) = 1 - C_E - \frac{1}{1+a} + \sum_{n=2}^{\infty} (-1)^n [\zeta(n-1)] a^{n-1}, \quad |a| < 1, \quad (77)$$

where ζ is the Riemann zeta function, leads the corresponding power series for $\Re[\psi(1+ia)] = \Re[\psi(ia)]$:

$$\Re[\psi(ia)] = 1 - C_E - \frac{1}{1+a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] a^{2n}, \quad |a| < 2, \quad (78)$$

and the function $f(a) = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}$ can be represented as

$$\begin{aligned} f(a) &= 1 - \frac{1}{1+a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] a^{2n}, \quad |a| < 2, \quad (79) \\ &= 1 - \frac{1}{1+a^2} + 0.2021 a^2 - 0.0369 a^4 + 0.0083 a^6 - \dots \end{aligned}$$

A equivalent way to estimate $f(a)$ to four decimal signs, is to present the sum from (59) in the following form [17]:

$$\begin{aligned} \sum &= (1+a^2)^{-1} + \sum_{n=1}^{\infty} (-a^2)^{n-1} [\zeta(2n+1) - 1], \quad (80) \\ &= (1+a^2)^{-1} + 0.20206 - 0.0369 a^2 + 0.0083 a^4 - 0.002 a^6. \end{aligned}$$

Eq. (80) is sufficient to evaluate this sum up to $a < 2/3 = 0.667$.

The calculation results for (79) and (80), relative CC and their difference with the Molière corrections are given in Table 2. Some results from Tables 1,2 illustrates Figure 1.

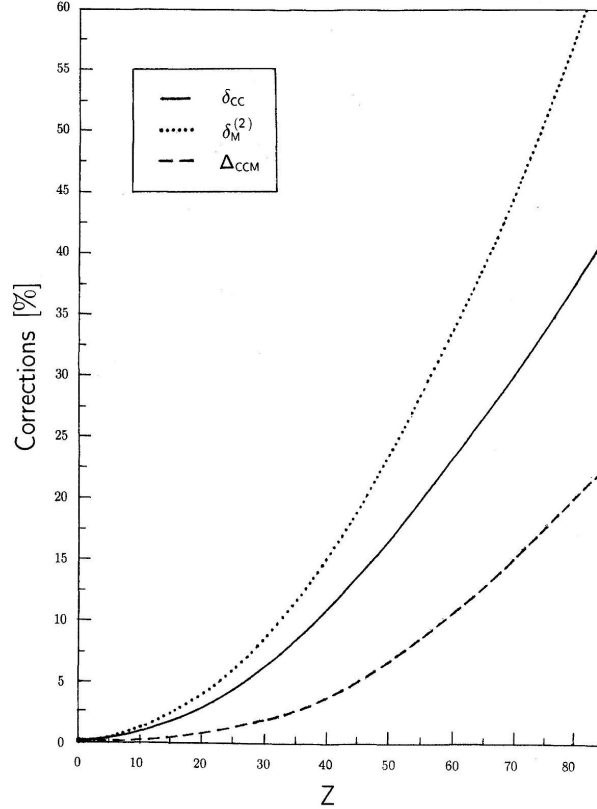


Figure 1: The dependence of the relative Coulomb (δ_{CC}) and Molière ($\delta_M^{(2)}$) corrections, and their difference (Δ_{CCM}) from nuclear charge Z .

It will be seen from Table 2 that for the light elements up to $Z = 28$, all the exact corrections coincide with the corresponding second-order corrections of Table 1. Beginning with $Z = 42$, the relative CC are lower than above-mentioned $\delta_{CC}^{(2)}(\chi'_a) > \delta_{CC}(\chi'_a)$, and this discrepancy increases approximately to 10% for the heavy elements with $Z \sim 80$. The magnitude of $\Delta_{CC} [\ln(\chi'_a)]$ from (61) is reached for $Z \sim 80$ the value of order of 30%. The size of the corresponding relative CC for these values of Z is approximately 40%. The absolute and relative differences with Molière corrections at $Z \sim 80$ are about 20% and 34%, respectively.

Thus, in the case of scattering on targets with large Z the such corrections as $\delta_{CC}(\chi'_a)$ and $\Delta_{CCM}(\chi'_a)$ become significant and should be taken into account in determining the lifetimes of relativistic elementary atoms in experiments with nuclear targets (see, e.g., [3]).

The application of formulas (60), (61) to the Migdal theory of the Landau—Pomeranchuk—Migdal effect, allowed to agree the results of theory and on experiment, was considered in [23].

7 Conclusions

1. We have obtained the rigorous relations for the first-order Born and exact values of the quantities $Q(\eta)$, $\ln[g(\eta)]$, and χ'_a , which do not depend on the shape of the electron density distribution in the atom and are valid for any atomic model.
2. We also calculated the Coulomb corrections $\Delta_{CC} \equiv \Delta_{CC}[\ln(\chi'_a)] = \Delta_{CC}[\ln g(\chi_c)]$ and relative corrections $\delta_{CC} \equiv \delta_{CC}(\chi'_a) = \delta_{CC}[g(\chi_c)] = \delta_{CC}[W_M(\chi_c, t)]$ with nuclear charge ranged from $Z = 2$ to $Z = 82$ and showed that for $Z = 28$ these correction are approximately 5 percent, and their maximum values for $Z \sim 80$ comprise the order of 30 percent and 40 percent, correspondingly.
3. Additionally, we evaluated absolute and relative accuracies of the Molière theory in determining the screening angle χ'_a . In particular, we concluded that for a target material, which intended to be used in the DIRAC experiment, these corrections are about 2 and 29 percents in the case of a Ni target ($Z = 28$), and they amounts to 16 and 33 percents, respectively, for a tantalum target ($Z = 73$).

Acknowledgments

One of the authors is grateful to Dr. Leonid Afanasyev, who initiated the consideration of the problem discussed in this paper.

Appendix: Approximate solution for the thick targets

We can also obtain the approximate solution (21) of Eq. (7) for the thick targets in the following simple way. If the total number of collisions is

$$N_0 = 2\pi n_0 t \int_0^\infty \sigma(\chi) \chi d\chi \gg 1, \quad (81)$$

then at small angles like $\chi_0 \eta \ll 1$, we can write

$$1 - J_0(\chi\eta) \approx \frac{\chi^2 \eta^2}{4}, \quad (82)$$

which will make it possible to reduce the integral (7) to a much simpler one:

$$W_M(\theta, t) = \int_0^\infty \eta d\eta J_0(\theta\eta) \exp \left[-2\pi n_0 t \frac{\eta^2}{4} \int_0^\infty \sigma(\chi) \chi^3 d\chi \right]. \quad (83)$$

In view of the that

$$\lim_{\chi \rightarrow \infty} \sigma(\chi) \chi^3 \rightarrow 0, \quad (84)$$

the corresponding integrand from (83) is a convergent integral

$$\int_0^\infty \sigma(\chi) \chi^3 d\chi < \infty, \quad (85)$$

and the integration of (83), using the fact

$$\int_0^\infty d\eta \eta J_0(\theta\eta) = 2c^{-2} \frac{\Gamma(1)}{\Gamma(0)} = 0, \quad (86)$$

where $\Gamma(x) = (x-1)!$ is the Euler Gamma function [24], yields the final result:

$$W_M(\theta, t) \approx \frac{2}{\bar{\theta}^2} \exp \left(-\frac{\theta^2}{\bar{\theta}^2} \right) \quad (87)$$

with

$$\bar{\theta}^2 = 2\pi n_0 t \int \sigma(\chi) \chi^3 d\chi. \quad (88)$$

For the Rutherford law

$$\sigma^R(\chi) = \left(\frac{2Z\alpha}{\beta p} \right)^2 \frac{1}{\chi^4} \quad (89)$$

at large angles, when $\sigma^R(\chi) \gg \theta_0 = \chi_0$, the quantity (88) take on a value

$$\bar{\theta}^2 = 2\pi n_0 t \int \sigma(\chi) \chi^3 d\vartheta = \infty, \quad (90)$$

and the approximate solution (87), as well as (21), is not applicable.

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